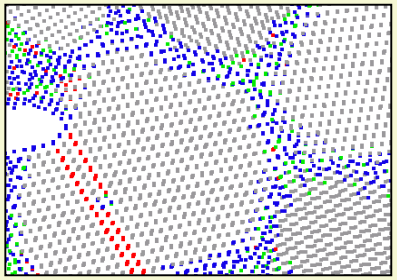
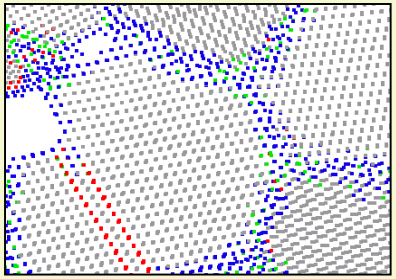
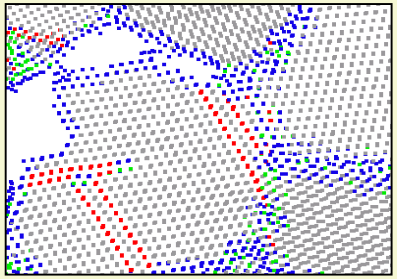
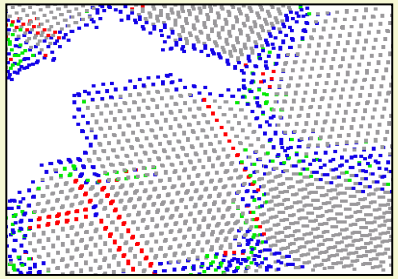
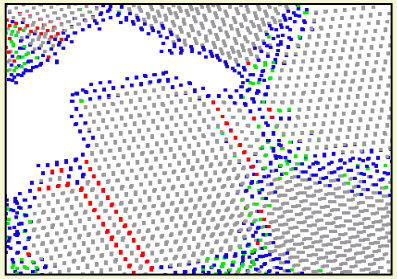










Computer Simulation of Fracture and Deformation Behavior of Nanocrystalline Metallic Materials Award Number: 0243947

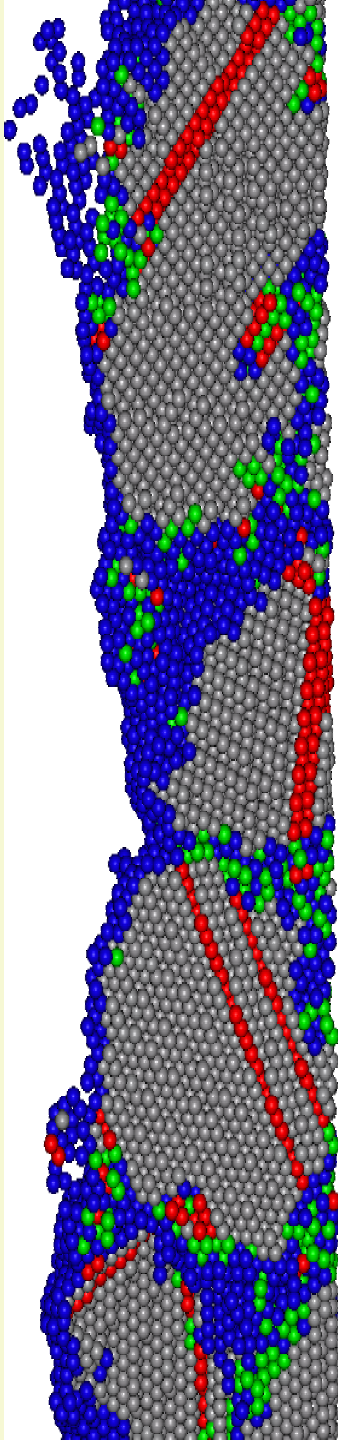
Diana Farkas Virginia Tech, diana@vt.edu

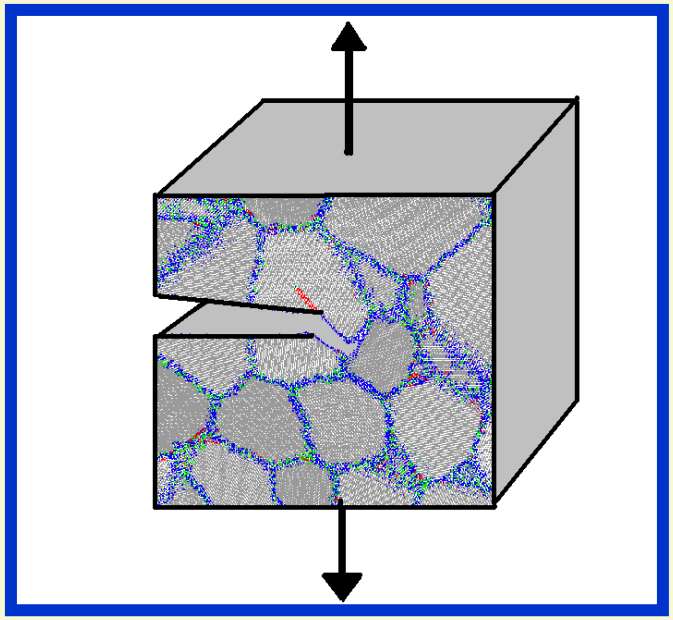
•The research addresses fundamental questions in the area of fracture and deformation of nanocrystalline materials.

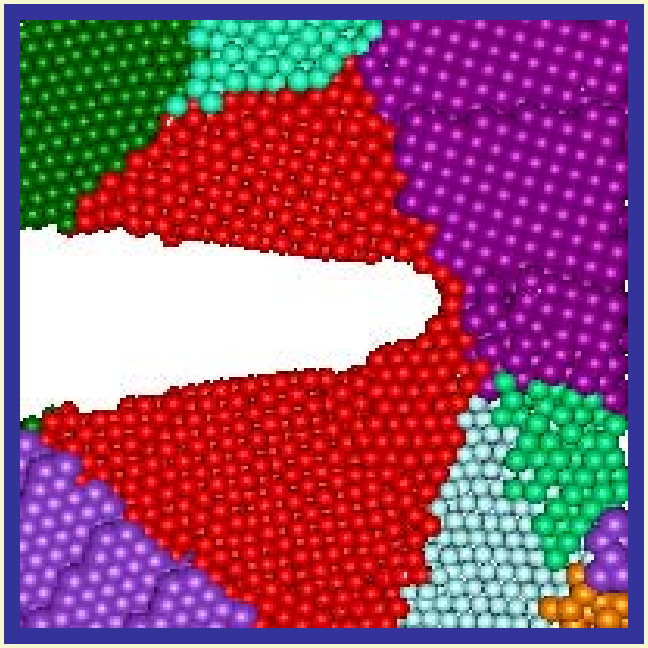
•We have found an intergranular fracture mechanism for nanocrystalline Ni modeled using fully 3D atomistic techniques. The figures left show the crack propagation mechanisms, dislocation activity is indicated in red.

•The figure to the right shows the shape of the crack front observed as the crack advances.

•The energetics of crack propagation as a function of the nano-grain size are also obtained from the simulations







•This activity also involves graduate level education and exposure to the broader international scientific community. This NSF project is co-funded by the Office of Multidisciplinary Activities, the Division of Materials Research, and the International Office (Western Europe) as a Cooperative Activity in Materials Research between the NSF and Europe This project is being carried out in collaboration with the Paul Scherrer Institute, Switzerland.

•The research results are being incorporated into the curriculum in graduate courses on fracture mechanics The results are being used as examples in the teaching of the role of interfaces in the fracture behavior on nanocrystalline materials

•The illustrations left are used to illustrate crack deviation and propagation along grain boundaries (top) and crack arrest at grain boundaries (bottom)